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From:	Zeman, Mary
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Subject:	Text search 10/655870

Please perform a text search of the following claim of 10/655870

A method for calculating a potential of mean force (PMF) score of a protein-ligand complex, the method comprising:
accessing one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex, the one or more parameters corresponding to an atom-pair type of the protein-ligand atom pair;
using the one or more accessed parameters, calculating the repulsion term useable to calculate the PMF of the protein-ligand atom pair; and
communicating the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.

Key terms: potential of mean force (PMF); repulsion; parameter; protein; ligand

Inventors:

Last name, First name:		City:	Country or State:
PURVIS	GEORGE	BEAVERTON	OREGON

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Paper printout please
Thanks, MKZ

Mary K. Zeman
Primary Examiner, 1631
571-272-0723
Remsen 2D61
MAILBOX: REM 2C70
mary.zeman@uspto.gov